

Macroscopic current fluctuations in stochastic lattice gases

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We study current fluctuations in lattice gases in the macroscopic limit extending the dynamic approach to density fluctuations developed in previous articles. More precisely, we derive large deviation estimates for the space-time fluctuations of the empirical current which include the previous results. Large time asymptotic estimates for the fluctuations of the time average of the current, recently established by Bodineau and Derrida, can be derived in a more general setting. There are models where we have to modify their estimates and some explicit examples are introduced.

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In a series of recent papers [1, 2, 3] we have developed a dynamical approach to macroscopic fluctuations of thermodynamic variables in non equilibrium steady states of stochastic lattice gases. The main object studied in these papers is the empirical density for which we established a large deviation principle. From this principle we obtained several results: we have shown that the entropy functional satisfies a Hamilton–Jacobi equation, we have extended Onsager–Machlup theory [4] and the minimum dissipation principle [5] to stationary non equilibrium states.

Another observable of great physical interest is the macroscopic current flowing through the system [6, 7, 8, 9, 10]. In the present article we develop, in the same spirit of [1, 2], a large deviation principle for the empirical current and discuss some of its consequences. We discuss the asymptotic probability, as the number of degrees of freedom increases, of observing a space-time dependent current profile different from the typical value. This new principle includes the previous one for the density and leads to a unified approach to fluctuations in steady states both equilibrium and non equilibrium. From this asymptotics we derive a more general form of a large fluctuation principle recently obtained by Bodineau and Derrida [11] for the large time fluctuations of the time averaged current. We show that there are models where one has to replace the large deviation functional obtained in [11], that we denote by $U(J)$, by its convex envelope $U^{**}(J)$. We discuss some examples where $U^{**} < U$; this is naturally interpreted as a dynamical phase transition. However more complex situations are also conceivable.

In a forthcoming more detailed paper [12] we shall study also the behavior of the current large deviation functional under time reversal and connect it to the well known fluctuation theorem for entropy production of Gallavotti and Cohen [13, 14, 15].

As the basic microscopic model we consider a stochastic lattice gas with a weak external field and particle

reservoirs at the boundary. More precisely, let $\Lambda \subset \mathbb{R}^d$ be a smooth domain and set $\Lambda_N = N\Lambda \cap \mathbb{Z}^d$; we consider a Markov process on the state space X^{Λ_N} , where X is a subset of \mathbb{N} , e.g. $X = \{0, 1\}$ when an exclusion principle is imposed. The number of particles at the site $x \in \Lambda_N$ is denoted by $\eta_x \in X$ and the whole configuration by $\eta \in X^{\Lambda_N}$. The dynamics of the particles is described by a continuous time Markov process on the state space X^{Λ_N} with transition rates $c_{x,y}(\eta)$ from a configuration η to $\sigma^{x,y}\eta$ that is the configuration obtained from η by moving a particle from x to a nearest neighbor site y . Similar rates c_x^\pm describe the appearance or loss of a particle at the boundary site x . The reservoirs are characterized by a chemical potential γ . We assume that the rates satisfy the local detailed balance condition [15] with respect to a Gibbs measure associated to some Hamiltonian \mathcal{H} . Typically, for a non equilibrium model, we can consider Λ the cube of side one and the system under a constant force E/N . Moreover we choose the chemical potential γ so that $\gamma(y/N) = \gamma_0$ if the first coordinate of y is 0, $\gamma(y/N) = \gamma_1$ if the first coordinate of y is N , and impose periodic boundary conditions in the other directions of Λ .

The fluctuation theory of stochastic lattice gases, as discussed below, is expected to apply to a wider class of non equilibrium systems with conservation laws. For instance, the Hamiltonian system discussed in [16] is reduced to the analysis of a Markov process. We introduce the empirical density π^N associated to a microscopic configuration $\eta \in X^{\Lambda_N}$ by requiring for each smooth function $G : \Lambda \rightarrow \mathbb{R}$,

$$\langle \pi^N, G \rangle = \int_{\Lambda} du \pi^N(u) G(u) = \frac{1}{N^d} \sum_{x \in \Lambda_N} G(x/N) \eta_x$$

so that $\pi^N(u)$ is the local density at the macroscopic point $u = x/N$ in Λ .

Consider a sequence of initial configurations η^N such that $\pi^N(\eta^N)$ converges to some density profile ρ_0 . Under

diffusive scaling the empirical density at time t converges, as $N \rightarrow \infty$, to $\rho = \rho(t, u)$ which is the solution of

$$\partial_t \rho = \nabla \cdot \left[\frac{1}{2} D(\rho) \nabla \rho - \chi(\rho) \nabla V \right] = \mathcal{D}(\rho) \quad (1)$$

with initial condition ρ_0 . Here D is the diffusion matrix, given by the Green–Kubo formula, see [17, II.2.2], χ is the conductivity, obtained by linear response theory, see [17, II.2.5], and ∇V the external field. We emphasize that these transport coefficient are defined in terms of the equilibrium Gibbs measure. In particular if we denote by $S_0(\rho)$ the entropy associated to \mathcal{H} , the usual Einstein relation $D(\rho) = R^{-1}(\rho) \chi(\rho)$ holds, here $R(\rho) = S_0''(\rho)^{-1}$ is the compressibility. The interaction with the reservoirs appears as a boundary condition to be imposed on solutions of (1). More precisely, we require that $S_0''(\rho(u)) = \gamma(u)$, $u \in \partial\Lambda$, here $\partial\Lambda$ denotes the boundary of Λ and we recall that γ is the chemical potential of the reservoirs. The non equilibrium stationary profile $\bar{\rho}$ is the unique stationary solution of (1).

Denote by μ^N the non equilibrium stationary ensemble, i.e. the invariant measure of the microscopic process. The probability of density fluctuations can be described, for large N , by an entropy functional $S(\rho)$ which depends on the local density of particles ρ . The stationary profile $\bar{\rho}$ corresponds to a critical point of S so that it is a minimum of the entropy; here we use the probabilist sign convention for S which is opposite to physicist convention. Hereafter, we normalize the entropy $S(\rho)$ so that $S(\bar{\rho}) = 0$. As shown in [1, 2], the entropy functional S satisfies the following Hamilton–Jacobi functional derivative equation

$$\frac{1}{2} \left\langle \nabla \frac{\delta S}{\delta \rho}, \chi(\rho) \nabla \frac{\delta S}{\delta \rho} \right\rangle + \left\langle \frac{\delta S}{\delta \rho}, \mathcal{D}(\rho) \right\rangle = 0 \quad (2)$$

where $\langle \cdot, \cdot \rangle$ means integration with respect to the space variable $u \in \Lambda$. It shows that once we know the hydrodynamic equation, we can obtain a closed macroscopic description.

The probability to observe a macroscopic trajectory different from the hydrodynamic behavior (1) is exponentially small in N^d and given by

$$\mathbb{P}_\mu^N(\pi^N \approx \rho, t \in [0, T]) \sim \exp \{ -N^d I_{[0, T]}(\rho) \} \quad (3)$$

where \approx denotes closeness in some metric, \sim logarithmic equivalence as $N \rightarrow \infty$, and \mathbb{P}_μ^N stands for the distribution of the stationary process, namely we consider an initial condition distributed according to the invariant measure μ^N . The rate functional $I_{[0, T]}(\rho)$ is given by

$$I_{[0, T]}(\rho) = S(\rho(0)) + \frac{1}{2} \int_0^T dt \langle \nabla H, \chi(\rho) \nabla H \rangle \quad (4)$$

where the external potential H has to be chosen so that ρ solves

$$\partial_t \rho = \mathcal{D}(\rho) - \nabla \cdot (\chi(\rho) \nabla H) \quad (5)$$

with the same boundary conditions as the hydrodynamic equation (1). Equations (3)–(5) represent a dynamical generalization of Einstein formula for thermodynamic fluctuations.

We give now a parallel discussion for the current. Denote by $\mathcal{N}_t^{x, y}$ the number of particles that jumped from x to y in the macroscopic time interval $[0, t]$. Here we adopt the convention that $\mathcal{N}_t^{x, y}$ represents the number of particles created at y due to the reservoir at x if $x \notin \Lambda_N$, $y \in \Lambda_N$ and that $\mathcal{N}_t^{x, y}$ represents the number of particles that left the system at x by jumping to y if $x \in \Lambda_N$, $y \notin \Lambda_N$. The difference $J_t^{x, y} = \mathcal{N}_t^{x, y} - \mathcal{N}_t^{y, x}$ represents the total current across the bond $\{x, y\}$ in the time interval $[0, t]$. In other words, given a path $\eta(s)$, $0 \leq s \leq t$, the instantaneous current $dJ_t^{x, y}/dt$ is a sum of δ -function localized at the jump times across the bond $\{x, y\}$ with weight $+1$, respectively -1 , if a particle jumped from x to y , respectively from y to x .

Fix a macroscopic time T and denote by \mathcal{J}^N the empirical measure on $[0, T] \times \Lambda$ associated to the current. For smooth vector fields $G = (G_1, \dots, G_d)$, the integral of G with respect to \mathcal{J}^N , denoted by $\mathcal{J}^N(G)$, is given by

$$\begin{aligned} \mathcal{J}^N(G) &= \int_0^T dt \int_\Lambda du G(t, u) \cdot \mathcal{J}^N(t, u) \\ &= \frac{1}{N^{d+1}} \sum_{i=1}^d \sum_x \int_0^T dt G_i(t, x/N) \frac{dJ_t^{x, x+e_i}}{dt} \end{aligned}$$

where \cdot is the inner product in \mathbb{R}^d , e_i is the canonical basis, and we sum over all x such that either $x \in \Lambda_N$ or $x + e_i \in \Lambda_N$. We normalized \mathcal{J}^N so that it is finite as $N \rightarrow \infty$.

Given a density profile ρ let us denote by

$$J(\rho) = -\frac{1}{2} D(\rho) \nabla \rho + \chi(\rho) \nabla V \quad (6)$$

the current associated to ρ . The hydrodynamic equation (1) can then be written as $\partial_t \rho + \nabla \cdot J(\rho) = 0$. If we consider an initial configuration η^N such that the empirical density $\pi^N(\eta^N)$ converges to some density profile ρ_0 and denote by $\rho(t)$ the solution of (1), then the empirical current $\mathcal{J}^N(t)$ converges, as $N \rightarrow \infty$, to $J(\rho(t))$, the current associated to the solution of the hydrodynamic equation (1). If we let the macroscopic time diverge, $t \rightarrow \infty$, we have $J(\rho(t)) \rightarrow J(\bar{\rho})$.

We next discuss the large deviation properties of the empirical current. Fix a smooth vector field $j : [0, T] \times \Lambda \rightarrow \mathbb{R}^d$ and a sequence of configurations η^N whose empirical density converges to some profile ρ_0 . The large deviation principle for the current states that

$$\mathbb{P}_{\eta^N}^N(\mathcal{J}^N(t, u) \approx j(t, u)) \sim \exp \{ -N^d \mathcal{I}_{[0, T]}(j) \} \quad (7)$$

where the rate function is given by

$$\mathcal{I}_{[0, T]}(j) = \frac{1}{2} \int_0^T dt \langle [j - J(\rho)], \chi(\rho)^{-1} [j - J(\rho)] \rangle \quad (8)$$

in which $J(\rho)$ is given by (6) and $\rho = \rho(t, u)$ is obtained by solving the continuity equation $\partial_t \rho + \nabla \cdot j = 0$ with initial condition $\rho(0) = \rho_0$. Of course there are compatibility conditions to be satisfied, for instance if we have chosen a j such that $\rho(t)$ becomes negative for some $t \in [0, T]$ then $\mathcal{I}_{[0, T]}(j) = +\infty$.

We present here a heuristic derivation of (7)–(8). Fix a current j ; in order to make j typical, we introduce an external field F . Let ρ be the solution of

$$\begin{cases} \partial_t \rho + \nabla \cdot j = 0 \\ \rho(0, u) = \rho_0(u) \end{cases} \quad (9)$$

and $F : [0, T] \times \Lambda \rightarrow \mathbb{R}^d$ be the vector field such that

$$\begin{aligned} j &= J(\rho) + \chi(\rho)F \\ &= -\frac{1}{2}D(\rho)\nabla\rho + \chi(\rho)\{\nabla V + F\} \end{aligned}$$

We introduce a perturbed measure $\mathbb{P}_{\eta_N}^{N, F}$ which is obtained by modifying the rates as follows

$$c_{x, y}^F(\eta) = c_{x, y}(\eta) e^{N^{-1}F(t, x/N) \cdot (y - x)}$$

Following a similar argument as the one for the large deviation principle of the empirical density [2], one can show that

$$\begin{aligned} \frac{d\mathbb{P}_{\eta_N}^N}{d\mathbb{P}_{\eta_N}^{N, F}} &\sim \exp \left\{ -N^d \frac{1}{2} \int_0^T dt \langle F, \chi(\rho)F \rangle \right\} \\ &= \exp \left\{ -N^d \mathcal{I}_{[0, T]}(j) \right\} \end{aligned}$$

Moreover, under $\mathbb{P}_{\eta_N}^{N, F}$, as $N \rightarrow \infty$, \mathcal{J}^N converges to j . Therefore,

$$\begin{aligned} \mathbb{P}_{\eta_N}^N \left(\mathcal{J}^N(t, u) \approx j(t, u), (t, u) \in [0, T] \times \Lambda \right) \\ = \mathbb{P}_{\eta_N}^{N, F} \left(\frac{d\mathbb{P}_{\eta_N}^N}{d\mathbb{P}_{\eta_N}^{N, F}} \mathbf{1}_{\{\mathcal{J}^N \approx j\}} \right) \sim e^{-N^d \mathcal{I}_{[0, T]}(j)} \end{aligned}$$

We emphasize that now we allow non-gradient external fields F , while in the large deviation principle for the empirical density (3), it is sufficient to consider gradient external fields [18, 19]. The latter is therefore a special case and can be recovered from (7)–(8).

We want to study the fluctuations of the time average of the empirical current over a large time interval $[0, T]$; the corresponding probability can be obtained from the space-time large deviation principle (7). Fix some divergence free vector field $J = J(u)$ constant in time and denote by $\mathcal{A}_{T, J}$ the set of all currents j such that $T^{-1} \int_0^T dt j(t, u) = J(u)$. The condition of vanishing divergence on J is required by the local conservation of the number of particles. By the large deviations principle (7), for T large we have

$$\mathbb{P}_{\eta_N}^N \left(\frac{1}{T} \int_0^T dt \mathcal{J}^N(t) \approx J \right) \sim \exp \left\{ -N^d T \Phi(J) \right\} \quad (10)$$

where the logarithmic equivalence is understood by sending *first* $N \rightarrow \infty$ and *then* $T \rightarrow \infty$. In [12] we show that for the so-called zero range process the limits can be taken in the opposite order; we expect this to be true in general. The functional Φ is given by

$$\Phi(J) = \lim_{T \rightarrow \infty} \inf_{j \in \mathcal{A}_{T, J}} \frac{1}{T} \mathcal{I}_{[0, T]}(j) \quad (11)$$

By a standard sub-additivity argument it is indeed easy to show the limit exists. We now prove that Φ is a convex functional. Let $J = pJ_1 + (1-p)J_2$: we want to show that $\Phi(J) \leq p\Phi(J_1) + (1-p)\Phi(J_2)$. Let us call $(j_1(t), \rho_1(t))$, $t \in [0, pT]$ (respectively $(j_2(t), \rho_2(t))$, $t \in [0, (1-p)T]$) the optimal path of current and density which implements the inf in (11) at J_1 (resp. J_2). We then consider a path $(j(t), \rho(t))$ which spends a time interval pT following (j_1, ρ_1) and a time interval $(1-p)T$ following (j_2, ρ_2) (and a finite time to go continuously from (j_1, ρ_1) to (j_2, ρ_2)). With such a path we get

$$\begin{aligned} \Phi(J) &\leq \frac{1}{T} \mathcal{I}_{[0, pT]}(j_1) + \frac{1}{T} \mathcal{I}_{[0, (1-p)T]}(j_2) \\ &\leq p\Phi(J_1) + (1-p)\Phi(J_2) + \epsilon \end{aligned}$$

In the last step we used the existence of the limit (11).

We next study the variational problem on the right hand side of (11). We begin by deriving an upper bound. Given $\rho = \rho(u)$ and $J = J(u)$, $\nabla \cdot J = 0$, let us introduce the functionals

$$\mathcal{U}(\rho, J) = \frac{1}{2} \langle J - J(\rho), \chi(\rho)^{-1} [J - J(\rho)] \rangle \quad (12)$$

$$U(J) = \inf_{\rho} \mathcal{U}(\rho, J) \quad (13)$$

where the minimum in (13) is carried over all profiles ρ satisfying the boundary conditions and $J(\rho)$ is given by (6). When J is constant, that is in the one-dimensional case, the functional U is the one introduced in [11].

By choosing a suitable path $j(t, u) \in \mathcal{A}_{T, J}$ we first show that

$$\Phi(J) \leq U(J) \quad (14)$$

The strategy is quite simple. Let $\hat{\rho} = \hat{\rho}(J)$ be the density profile which minimizes the variational problem (13). Given the initial density profile ρ_0 , we construct a path $j = j(t, u)$, $(t, u) \in [0, T] \times \Lambda$ as follows

$$j(t) = \begin{cases} \hat{j} & \text{if } 0 \leq t < \tau \\ \frac{T}{T-2\tau} J & \text{if } \tau \leq t < T - \tau \\ -\hat{j} & \text{if } T - \tau \leq t \leq T \end{cases}$$

where \hat{j} is a vector field such that $\tau \nabla \cdot \hat{j} = \rho_0 - \hat{\rho}$ and $\tau > 0$ is some fixed time. It is now straightforward to verify that $j \in \mathcal{A}_{T, J}$, as well as $\lim_{T \rightarrow \infty} \frac{1}{T} \mathcal{I}_{[0, T]}(j) = U(J)$.

From (14) and the convexity of $\Phi(J)$ it immediately follows that

$$\Phi(J) \leq U^{**}(J) \quad (15)$$

We next discuss a lower bound for the variational problem (11). We denote by \tilde{U} and \tilde{U} the same functionals as in (12)–(13), but now defined on the space of all currents without the conditions of vanishing divergence. Let also \tilde{U}^{**} be the convex envelope of \tilde{U} .

Let $j \in \mathcal{A}_{T,J}$, by the convexity of \tilde{U}^{**} in the set of all currents, we get

$$\begin{aligned} \frac{1}{T} \mathcal{I}_{[0,T]}(j) &= \frac{1}{T} \int_0^T dt \tilde{U}(\rho(t), j(t)) \geq \frac{1}{T} \int_0^T dt \tilde{U}(j(t)) \\ &\geq \frac{1}{T} \int_0^T dt \tilde{U}^{**}(j(t)) \geq \tilde{U}^{**}(J) \end{aligned} \quad (16)$$

The upper and lower bounds (15) and (16) are, in general, different. For a divergence free J we have $\tilde{U}(J) = U(J)$ but since the convex envelopes are considered in different spaces, we only have $\tilde{U}^{**}(J) \leq U^{**}(J)$.

To understand the physical meaning of the convex envelope in (15), suppose $J = pJ_1 + (1-p)J_2$ and $U(J) > U^{**}(J) = pU(J_1) + (1-p)U(J_2)$ for some p, J_1, J_2 . The values p, J_1, J_2 are determined by J and U . In addition we assume that $U^{**} = \tilde{U}^{**}$. If we condition on observing an average current J , the corresponding density profile is not determined, but rather we observe with probability p the profile $\hat{\rho}(J_1)$ and with probability $1-p$ the profile $\hat{\rho}(J_2)$. When U is not convex we have thus a situation in which the time averaged current J is realized with the coexistence of two dynamical regimes: we have a dynamical phase transition.

The derivation of the upper bound shows that, if U is not convex, our result differs from the one in [11]. On the other hand if $\tilde{U}^{**}(J) < U^{**}(J)$ it is possible that one can improve it by exploring currents with non vanishing divergence. In such a situation it is not clear to us if Φ can be directly related to U .

We can consider the large time behavior of the empirical current as in equation (10) with the additional constraint that the associated density is asymptotically time independent. In such a case it is not difficult to show that (10) holds with $\Phi = U$. With this extra constraint we are in fact forbidding the system from oscillating.

In the models where the diffusion coefficient $D(\rho)$ is constant and the mobility $\chi(\rho)$ is concave, for example in the symmetric simple exclusion where $\chi = \rho(1-\rho)$, it is not difficult to see that \tilde{U} is convex. Therefore in these cases $\Phi = U$. In [12] we shall show that in the Kipnis-Marchioro-Presutti model [20, 21] at equilibrium $U(J)$ is convex while $\tilde{U}(J)$ is not.

We next discuss an example, with a non-concave χ , where the functional U is not convex. We fix equilibrium boundary conditions $\rho_0 = \rho_1 = \bar{\rho}$. We take $D(\rho) = 1$ and $\chi(\rho)$ a smooth function with $\chi(0) = \chi(1) = 0$ which

has a non concave part $\chi(\rho) = Ke^{-C\rho}$, for ρ in a given interval, where C is a positive parameter. An explicit calculation gives that

$$U(J) = \frac{1}{C^2} e^{C\bar{\rho}} F(CJ) \quad (17)$$

where $F(z) = z \frac{e^z - 1}{e^z + 1}$, if J is in an appropriate interval. Since the second derivative of $F(z)$ can be negative, $U(J)$ is not convex.

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